

**Title:** Comparative Developmental Toxicity of a Comprehensive Suite of Polycyclic Aromatic Hydrocarbons

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**Authors:** Mitra C. Geier, Anna C. Chlebowski, Lisa Truong, Staci L. Massey Simonich, Kim A. Anderson, Robert L. Tanguay\*

Department of Environmental and Molecular Toxicology, Oregon State University, ALS 1007, Corvallis, OR 97331

\* Correspondence to:

Robert Tanguay, Ph.D. Department of Environmental and Molecular Toxicology, the Sinnhuber Aquatic Research Laboratory 28645 East Highway 34, Oregon

State University, Corvallis, OR 97333. Email: Robert.Tanguay@oregonstate.edu, Telephone: 1-541-737-6514, Fax: 1-541-737-6074

**Table S1** Lowest effect levels for morphological endpoints (uM)

| Compound                 | 120 Notochord | 120 Swim Bladder | 120 Trunk | Circulation | Pigmentation | Caudal Fin | Touch Response |
|--------------------------|---------------|------------------|-----------|-------------|--------------|------------|----------------|
| 1,2-dimethylnaphthalene  |               |                  |           |             |              |            |                |
| 1,2-naphthoquinone       | 5             |                  |           |             |              |            |                |
| 1,3-dihydroxynaphthalene |               |                  |           |             |              |            |                |
| 1,3-dinitropyrene        | 0.1           | 0.1              |           | 1.12        | 0.5          | 0.5        | 0.1            |
| 1,4-antraquinone         | 1.12          | 1.12             | 3.56      |             | 3.56         |            | 1.12           |
| 1,4-dimethylnaphthalene  |               |                  |           |             |              |            |                |
| 1,4-phenanthrenedione    |               | 1.12             | 1.12      |             | 0.5          |            |                |
| 1,5-dihydroxynaphthalene | 35.6          | 50               |           | 35.6        | 50           | 50         | 50             |
| 1,5-dimethylnaphthalene  |               |                  |           |             |              |            |                |
| 1,6-dihydroxynaphthalene |               |                  |           |             |              |            |                |
| Any Except Mortality     |               |                  |           |             |              |            |                |
| Any Effect               |               |                  |           |             |              |            |                |







|                            |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|----------------------------|------|------|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Naphtho[2,3-k]fluoranthene |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Perinaphthenone            | 5    | 5    | 50   |      |  | 35.6 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 11.2 | 5    | 11.2 | 11.2 |
| Phenanthrene               |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Pyrene                     | 50   | 50   |      |      |  | 50   | 50   |      |      |      |      | 50   |      |      | 50   |      |      |      |      |      | 50   |
| Pyrene-4,5-dione           | 1.12 | 1.12 | 3.56 |      |  | 3.56 |      | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 |      |
| Quinoline                  |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Retene                     | 11.2 | 11.2 | 50   | 35.6 |  | 35.6 | 35.6 | 11.2 | 11.2 | 11.2 | 11.2 |      | 11.2 |      |      | 11.2 |      | 11.2 |      |      |      |
| Thianaphthene              |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Triphenylene               |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Xanthene                   |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Xanthone                   | 35.6 | 35.6 |      |      |  |      | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   | 50   |      |

**Table S2** Direction of significant changes in EPR behavior, for compounds with significant behavior effects in at least one phase. + indicates hyperactive, - indicates hypoactive compared to the controls, NA denotes phases that were not significantly different from controls in all tested concentrations.

| Compound                 | Baseline | Excitation | Recovery |
|--------------------------|----------|------------|----------|
| 1,3-dinitropyrene        | +        | +          | NA       |
| 1,4-antraquinone         | -        | NA         | NA       |
| 1,4-phenanthrenedione    | -        | -          | NA       |
| 1,8-dinitropyrene        | NA       | +          | NA       |
| 1-aminoypyrene           | -        | -          | NA       |
| 1-hydroxyphenanthrene    | NA       | -          | NA       |
| 1-hydroxypyrene          | NA       | +          | NA       |
| 2,3-dihydroxynaphthalene | +        | +          | NA       |
| 2-nitrobenzothiophene    | NA       | -          | NA       |
| 2-nitrofluorene          | NA       | -          | NA       |
| 3,6-dimethylphenanthrene | NA       | -          | NA       |
| 3-hydroxybenzo[e]pyrene  | -        | -          | NA       |
| 3-hydroxyfloranthene     | NA       | -          | NA       |
| 3-hydroxyphenanthrene    | -        | -          | NA       |
| 3-nitrobenzanthrone      | -        | -          | NA       |
| 4-hydroxychrysene        | NA       | -          | NA       |
| 4-hydroxyphenanthrene    | NA       | -          | NA       |
| 5,12-naphthacenequinone  | NA       | -          | NA       |

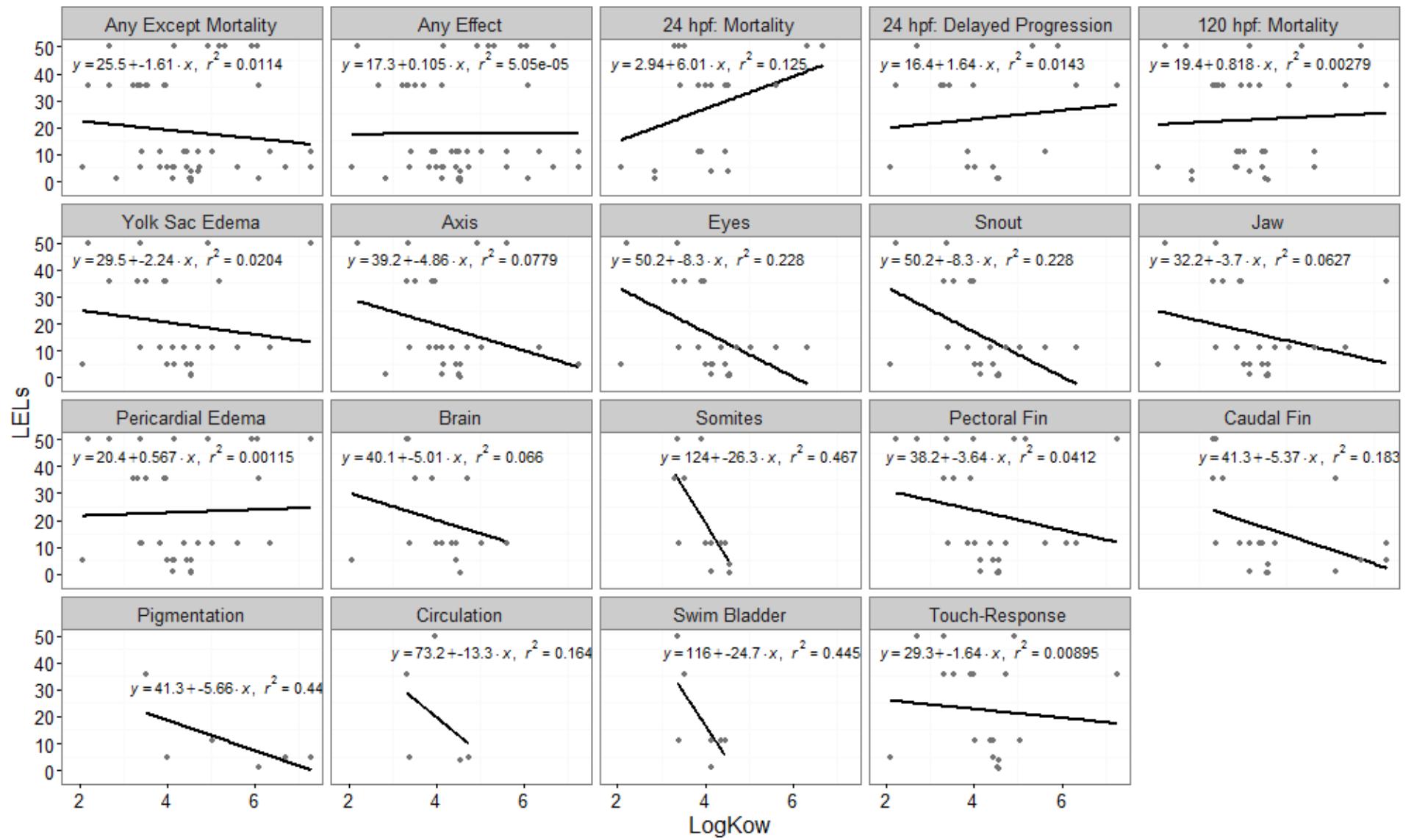
|                          |    |    |    |
|--------------------------|----|----|----|
| 9,10-phenanthrenequinone | -  | -  | NA |
| 9-aminophenanthrene      | NA | -  | NA |
| 9-hydroxyphenanthrene    | -  | -  | NA |
| Acenaphthenequinone      | NA | -  | NA |
| Benzanthrone             | NA | -  | NA |
| Dibenzo[a,h]pyrene       | NA | NA | -  |
| Pyrene-4,5-dione         | -  | NA | NA |
| Quinoline                | NA | +  | NA |
| Retene                   | -  | -  | NA |
| Thianaphthene            | NA | +  | NA |

**Table S3** Direction of significant changes in LPR behavior, for compounds with significant behavior effects in at least one phase. + indicates hyperactive, - indicates hypoactive compared to the controls, NA denotes phases that were not significantly different from controls in all tested concentrations. “All” phase a comparison activity across the entire assay.

| Compound                         | All | Dark | Light |
|----------------------------------|-----|------|-------|
| 1,2-dimethylnaphthalene          | +   | +    | NA    |
| 1,2-naphthoquinone               | -   | -    | -     |
| 1,3-dihydroxynaphthalene         | +   | +    | +     |
| 1,3-dinitropyrene                | NA  | -    | +     |
| 1,4-antraquinone                 | +   | +    | +     |
| 1,4-dimethylnaphthalene          | +   | +    | +     |
| 1,4-phenanthrenedione            | NA  | -    | NA    |
| 1,5-dihydroxynaphthalene         | +   | NA   | -     |
| 1,5-dimethylnaphthalene          | NA  | -    | +     |
| 1,6-dihydroxynaphthalene         | NA  | +    | -     |
| 1,6-dimethylnaphthalene          | NA  | +    | -     |
| 1,8-dimethylnaphthalene          | NA  | +    | NA    |
| 1,8-dinitropyrene                | NA  | NA   | +     |
| 10-hydroxybenzo[a]pyrene         | NA  | NA   | +     |
| 1-aminopyrene                    | NA  | NA   | +     |
| 1-hydroxyindeno[1,2,3-c,d]pyrene | +   | +    | NA    |
| 1-hydroxynaphthalene             | NA  | NA   | -     |
| 1-hydroxypyrene                  | +   | +    | +     |
| 1-methylnaphthalene              | +   | +    | NA    |
| 1-nitronaphthalene               | NA  | NA   | -     |
| 1-nitropyrene                    | -   | -    | +     |
| 2,3-dihydroxynaphthalene         | +   | +    | NA    |
| 2,3-dimethylanthracene           | NA  | NA   | +     |
| 2,6-dimethylnaphthalene          | -   | NA   | NA    |
| 2,7-dihydroxynaphthalene         | NA  | NA   | +     |
| 2,8-dinitrodibenzothiophene      | NA  | NA   | +     |
| 2-hydroxynaphthalene             | NA  | NA   | -     |
| 2-methylanthracene               | -   | NA   | -     |
| 2-methylnaphthalene              | -   | -    | +     |
| 2-nitrodibenzothiophene          | -   | -    | -     |

|  |    |    |    |
|--|----|----|----|
| 2-nitrofluoranthene                        | -  | NA | NA |
| 2-nitrofluorene                            | NA | NA | +  |
| 2-nitronaphthalene                         | NA | NA | +  |
| 3,6-dimethylphenanthrene                   | NA | -  | +  |
| 3,7-dinitrobenzo[k]fluoranthene            | +  | +  | NA |
| 3-hydroxybenz[a]anthracene                 | NA | NA | +  |
| 3-hydroxybenzo[e]pyrene                    | NA | -  | +  |
| 3-hydroxyfluorene                          | NA | -  | -  |
| 3-nitrodibenzofuran                        | NA | +  | -  |
| 3-nitrophenanthrene                        | NA | NA | -  |
| 4h-cyclopenta[def]phenanthren-4-one        | NA | -  | -  |
| 4H-cyclopenta[lmn]phenanthridine-5,9-dione | NA | NA | -  |
| 4-hydroxyphenanthrene                      | NA | NA | +  |
| 5,6-benzoquinoline                         | -  | -  | -  |
| 5-nitroacenaphthalene                      | NA | NA | +  |
| 6H-benzo[cd]pyren-6-one                    | -  | -  | -  |
| 6-methylchrysene                           | NA | -  | -  |
| 6-nitrochrysene                            | NA | NA | +  |
| 7-nitrobenz[a]anthracene                   | +  | +  | +  |
| 9-aminophenanthrene                        | NA | +  | NA |
| 9-anthracene carbonitrile                  | NA | NA | +  |
| 9-anthracene carboxylic acid               | NA | NA | +  |
| 9-fluorenone                               | +  | NA | +  |
| 9-hydroxyphenanthrene                      | NA | NA | +  |
| 9-methylanthracene                         | +  | +  | -  |
| 9-nitroanthracene                          | NA | NA | +  |
| 9-nitrophenanthrene                        | NA | NA | -  |
| acenaphthene                               | +  | +  | +  |
| acenaphthenequinone                        | NA | +  | +  |
| acenaphthylene                             | NA | NA | -  |
| acridine                                   | -  | NA | -  |
| anthanthrene                               | +  | NA | -  |
| anthraquinone                              | +  | +  | +  |
| benzanthrone                               | -  | -  | NA |

|                                |    |    |    |
|--------------------------------|----|----|----|
| benzo[a]pyrene                 | +  | NA | +  |
| benzo[b]fluoranthene           | -  | NA | -  |
| benzo[b]fluorene               | NA | NA | +  |
| benzo[c]phenanthrene[1,4]dione | NA | NA | -  |
| benzo[e]pyrene                 | +  | +  | -  |
| benzo[g,h,i]perylene           | +  | +  | +  |
| benzo[j]fluoranthene           | +  | +  | +  |
| carbazole                      | -  | -  | -  |
| chromone                       | +  | +  | -  |
| chrysene                       | +  | +  | -  |
| coronene                       | NA | +  | NA |
| dibenz[a,h]anthracene          | NA | +  | +  |
| dibenzo[a,h]pyrene             | +  | +  | -  |
| dibenzo[a,l]pyrene             | -  | NA | -  |
| dibenzo[b,k]fluoranthene       | +  | +  | +  |
| fluoranthene                   | NA | NA | +  |
| fluorene                       | +  | +  | NA |
| indeno[1,2,3-c,d]pyrene        | +  | NA | +  |
| indole                         | NA | NA | -  |
| naphthalene                    | +  | +  | +  |
| naphtho[1,2-b]fluoranthene     | NA | -  | NA |
| naphtho[2,3-e]pyrene           | +  | +  | +  |
| naphtho[2,3-j]fluoranthene     | NA | NA | +  |
| naphtho[2,3-k]fluoranthene     | NA | NA | -  |
| perinaphthenone                | NA | -  | NA |
| phenanthrene                   | +  | NA | +  |
| pyrene                         | -  | -  | +  |
| pyrene-4,5-dione               | +  | +  | NA |
| retene                         | NA | NA | -  |
| thianaphthene                  | NA | NA | -  |
| triphenylene                   | -  | +  | +  |
| xanthene                       | +  | +  | NA |
| xanthone                       | -  | -  | +  |



**Figure S1** Correlations between morphology endpoints and log  $K_{ow}$